

Diagnostic Characterization of Surface of Electrodes in High-Power Lithium-Ion Batteries using XPS and Infrared Spectroscopy

XueRong Zhang, Choongman Lee, and Philip N. Ross, Jr.
Materials Sciences Division
Lawrence Berkeley National Laboratory
University of California
Berkeley, California 94720

Introduction

The Advanced Technology Development (ATD) Program is a new effort by the U.S. Department of Energy (DOE) to aid the development of lithium-ion batteries for hybrid electric vehicle (HEV) applications. A baseline cell chemistry designed for high-power applications was identified as a carbon anode, $\text{LiNi}_x\text{Co}_{0.5}\text{Al}_2\text{O}_2$ based cathode and DEC-EC-LiPF₆ or EMC-EC-LiPF₆ electrolyte. Various diagnostic techniques were applied to determine cell component chemical, structural and morphological changes that lead to performance degradation and failure as they are aged, cycled and/or abused.¹ These diagnostic results are used to guide the improvement of cell chemistries. X-ray photoemission spectroscopy (XPS) and infrared spectroscopy (IR) are useful tools to analyze electrode surfaces. The diagnostic results from some ATD batteries cycled at different conditions using these two techniques are presented.

Experimental Section

Exsitu IR microscopy was conducted using a Nicolet Magna 760 with Nic-Plan IR Microscope in the LBNL Advanced Light Source. Airtight IR cells with KBr windows were constructed to perform IR microscopy on the air-sensitive and moisture-sensitive electrode materials. Electrode samples were harvested from various locations on the electrodes inside a dry box and then inserted into the IR cells, in order to preserve the electrode as it was in the battery. The electrode was washed in some XPS studies.

The base pressure of the chamber was less than 2×10^{-9} Torr. The excitation photons were created by a commercial dual anode (Mg/Mg) X-ray source operating at 15 kV and 400 W. The electrode sample is transferred into the UHV chamber in an air-free environment.

Results and Discussions

The electrolyte is reduced on the anode during the cell formation cycles and a solid state interface (SEI) layer is formed. Figure 1 shows the IR data of an anode sample from a cell undergone two formation cycles and one discharge. The broad peak at 1650 cm^{-1} is characteristic of C=O stretching of lithium alkylcarbonate, consistent with IR results of lithium ethyl carbonate synthesized in our lab and other literature report². A thin organic film (containing $-\text{H}_2\text{C}-\text{O}-$ and/or $-\text{HC}=\text{O}$ functionality), possibly a solvent oxidation product, was detected on the cathode surface

along with some LiF and Li_2CO_3 . A qualitative trend analysis of SEI formation for cells cycled under different conditions.

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References

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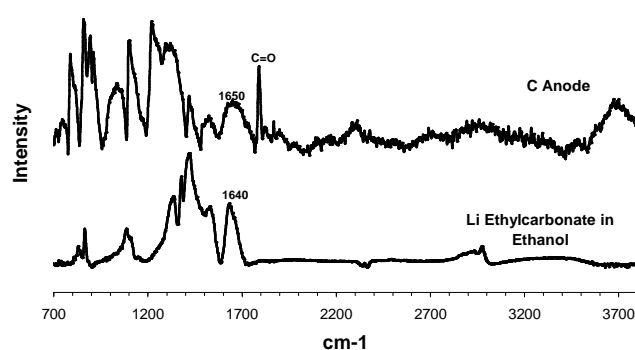


Figure 1